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Stochastic Simulation of Complex Fluid Flows

Aleksandar Donev
NEW YORK UNIVERSITY

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Air Force Research Laboratory
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70 WASHINGTON SQUARE S
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The PI has developed novel numerical algorithms and computational codes to simulate the Brownian motion of rigid particles immersed in a viscous fluid. This is crucial for modeling flowing colloidal suspensions of passive and active micro and nano particles, which is central to a number of industrial processes and to the design of novel nanofluid materials. The random Brownian motion of particles in fluid can be accounted for in fluid-structure coupling models via the framework of fluctuating hydrodynamics (FHD), which adds a stochastic component to the stress tensor. The PI has developed methods to couple rigid particles to a fluctuating fluid in the framework of the immersed boundary method.

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Aleksandar Donev, Courant Institute of Mathematical Sciences

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Summary

In this Young Investigator Program project, the PI and his students, postdocs and collaborators have developed novel numerical algorithms and computational codes to simulate the Brownian motion of rigid particles immersed in a viscous fluid. This is crucial for modeling flowing colloidal suspensions of passive and active micro and nano particles, which is central to a number of industrial processes and to the design of novel nanofluid materials. The random Brownian motion of particles in fluid can be accounted for in fluid-structure coupling models via the framework of fluctuating hydrodynamics (FHD), which adds a stochastic component to the stress tensor. The PI has developed methods to couple rigid particles to a fluctuating fluid in the framework of the immersed boundary method. In the first part of the project, work focused on minimially-resolved models for suspensions of spherical particles, and resulted in four publications in journals such as the Journal of Chemical Physics [1, 2, 3] and Computer Methods in Applied Mechanics and Engineering [4]. More recently, the PI has developed immersed-boundary methods for rigid bodies, and designed novel algorithms for simulating the translational and rotational Brownian motion of non-spherical rigid bodies, resulting in additional publications [5, 6]. The computer codes developed have been released as open source tools for other researchers to use, either as part of the mature open-source Immersed Boundary Adaptive Mesh Refinement (IBAMR) software framework [7], or through the PI's github page https://github.com/stochasticHydroTools.

Introduction

The presence of suspended particles is a common feature of complex fluids. At small scales, the motion of structures immersed in a viscous fluid is driven by thermal fluctuations, giving rise to Brownian motion, which is well-known to be strongly affected by hydrodynamic effects. Stochastic effects are important in flows at micro and nano scales typical of nano- and microfluidic and microelectromechanical devices, novel materials such as nanofluids, and biological systems such as lipid membranes, Brownian molecular motors, and nanopores.

In the limit of zero Reynolds number the methods of Brownian [8] and Stokesian dynamics [9] have dominated in chemical engineering, and related techniques have been used in biochemical engineering [10, 11]. These methods simulate the overdamped (diffusive) dynamics of the particles by using Green's functions for steady Stokes flow to capture the effect of the fluid. While this sort of implicit solvent approach works very well in many situations, it has several notable technical difficulties: achieving near linear scaling for many-particle systems is technically challenging, handling non-trivial boundary conditions (bounded systems) is complicated

and has to be done on a case-by-case basis, including thermal fluctuations is non-trivial, and generalizations to complex particle shapes is difficult.

In this work the PI and collaborators developed methods that couple an immersed boundary Lagrangian representation of rigid bodies to a fluctuating finite-volume fluid solver. Unlike commonly-used methods based on Green's functions, we rely on an explicit-fluid *fluctuating hydrodynamics* formulation in which we add a stochastic stress tensor to the usual viscous stress tensor. The underlying fluctuating hydrodynamics formulation automatically ensures the correct translational and rotational Brownian motion, more precisely, our methods ensure fluctuation-dissipation balance in the overdamped limit even in the presence of nontrivial boundary conditions. Complex rigid (e.g., synthetic nanorods) and semi-rigid (e.g., short DNA segments) particle shapes can be handled by composing each structure from a collection of spherical particles constrained to move (semi)rigidly.

Budget Report

The budgeted research funds were used essentially in their entirety. This YIP award fostered the development of the PI's research program by supporting course buyouts, summer research by the PI and his graduate students (Steven Delong and Bill Bao), attendance of key workshops and conferences in the field, and the hiring of qualified postdocs (Bakytzhan Kallemov and Florencio Balboa Usabiaga). The PI gave invited and plenary talks at several international and national meetings, including an invited presentation at the workshop on Fluid-Structure Interactions in Soft-Matter Systems held at the Monash University Prato Center, Italy, November 2012, as well as the workshop on Multiscale Simulation Methods for Soft Matter Systems, Mainz, Germany, October 2014. The PI also organized a minisymposium on *Hydrodynamics of Complex Fluids at the Micro and Nano-Scales* at the SIAM Conference on Computational Science and Engineering, held in Boston, MA, February 2013 and also Salt Lake City, UT, March 2015, as well as the SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, June 2013. The PI has recently been granted tenure at the Courant Institute of Mathematical Sciences at New York University.

Research Accomplishments

In the first two years substantial progress was made toward the objective to develop computational algorithms for simulating systems of interacting particles and structures immersed in a fluctuating fluid. We developed a minimally-resolved "blob" representation for Brownian particles suspended in fluid flow based on the immersed boundary method. First, we did this accounting for inertia of the fluid and the particles [4], i.e., for moderate Schmidt numbers as in nano-colloidal suspensions. We used this method to study previously unknown corrections to the Stokes-Einstein relation [1]. Next we extended this work to the overdamped (inertia-free or zero Reynolds number) limit [3], relevant for large Schmidt numbers as in suspensions of micron-sized particles, and developed a novel Fluctuating Immersed Boundary (FIB) method. Additionally, we have extended our minimally-resolved immersed boundary method approach to reaction-diffusion problems, enabling us to model chemically-propelled active Brownian particles [2]. We have developed numerical algorithms for these models and implemented them in the open-source IBAMR library (B. Griffith, NYU) [7]. Collaborations have been established with experimental groups at NYU (Paul Chaikin, Physics, and Michael Shelley, Courant) studying active suspensions of synthetic Brownian particles.

In the last year of the project we have made substantial progress toward extending the FIB method to suspensions of non-spherical rigid particles. The minimally-resolved blob approach cannot correctly describe the hydrodynamics of spherically-symmetric particles at short distances. It also cannot be used to describe the hydrodynamics for more complicated particle shapes such as nanorods. However, essentially arbitrary structures/bodies can be constructed by rigidly connecting a number of minimally-resolved (spherical) particles (blobs) to form what we call a *rigid multiblob [12]*. Importantly, the *level of resolution* can be increased from less to more resolved by increasing the number of blobs used to construct the rigid structure. This allows us to balance computational requirements with physical fidelity for each specific application.

So far, we have completed work on two key pieces required to enable rigid multiblob simulations that include both resolved hydrodynamics and Brownian motion. The first component was to account for the Brownian motion of particle orientations, including the challenging case when the hydrodynamic mobility (equivalently, resistance) functions depend strongly on the configuration. This is essential since in practice rigid particles diffuse either in a suspension, in which case they interact hydrodynamically with other particles, or near a boundary such as a microscope slip or the walls of a channel, in which case they interact hydrodynamically with the boundaries. This first component was developed in the last chapter of the Ph.D. thesis of student Steven Delong, who recently successfully defended his thesis "Temporal Integrators for Langevin Equations with Applications to Fluctuating Hydrodynamics and Brownian Dynamics" (available from the PI's home page). We are presently preparing a paper based on the thesis chapter [6], to be submitted shortly to J. Chem. Phys. In this work, we parameterize the orientation of the bodies using normalized quaternions, and construct a system of overdamped Langevin equations in the quaternion representation that accounts for hydrodynamic effects, preserves the unit-norm constraint on the quaternion, and is time reversible with respect to the Gibbs-Boltzmann distribution at equilibrium. We introduce two schemes for temporal integration of the overdamped Langevin equations of motion, one based on the Fixman midpoint method and the other based on a random finite difference approach, both of which ensure the correct stochastic drift term is captured in a computationally efficient way. We study several examples of rigid colloidal particles diffusing near a no-slip boundary, and demonstrate the importance of the choice of tracking point on the translational mean square displacement.

The second piece we have recently completed is the construction of immersed boundary methods for resolved rigid bodies. The challenge is that unlike the minimally-resolved models [4, 3], resolved rigid models require the imposition of a rigidity constraint on the fluid. This leads to a nontrivial linear algebra challenge that needed to be tackled. We recently successfully constructed a novel approach to rigid-body immersed boundary simulation [5]. Key features of our work are that we: (1) Do not employ time splitting and are thus suitable for the steady Stokes (viscous-dominated) regime; (2) Strictly enforce the rigidity constraint; and (3) Ensure fluctuation-dissipation balance in the overdamped limit even in the presence of nontrivial boundary conditions.

To our knowledge, in all prior work on rigid immersed bodies, what is lacking is a method to solve the constrained fluid problem both accurately and efficiently. In all prior work, accuracy is traded off to make the method reasonably efficient, usually by using time-splitting or by allowing for uncontrolled errors in imposing the rigidity constraints. This leads to splitting errors that can be acceptable at higher Reynolds number but that render the method unusable at low Reynolds numbers or for Stokes flows. In our recent paper [5] we show that we can

efficiently solve the constrained fluid problem to a desired target accuracy efficiently over the whole range of Reynolds numbers, including steady Stokes flow. The principal contribution of this paper is that it develops an efficient preconditioner for this exactly constrained IB formulation which is based on an analytical approximation to the Schur complement. Our method is able to give controlled accuracy with a controlled number of GMRES iterations for a broad range of Re numbers and boundary conditions.

Future Work

The work described above is only a partial step toward the ultimate goal of developing methods able to *efficiently* handle large numbers of rigid bodies/particles in low or moderate-number Reynolds number flow, including the steady Stokes limit (zero Reynolds number). Several computational challenges need to be tackled to realize this goal. Notably, it is crucial to extend the preconditioner developed in [5] to a large collection of *freely-moving* rigid bodies. Initial investigations have shown great promise in block-diagonal preconditioners with one block per body. In this approach, we neglect the hydrodynamic interactions between bodies, but use the mobility approximation developed in [5] together with dense linear algebra for each body.

Once we have the required spatial discretization and associated linear solvers for suspensions of moving rigid bodies, we need to include thermal fluctuations in the fluid stress and implement the temporal integrators developed in [6]. This will enable us to simulate Brownian motion in a confined suspension of nonspherical particles, a nontrivial accomplishment. We believe that our methods and codes will find many applications in chemical engineering and materials science.

In the marker-based immersed boundary (IB) method we have used in our work so far, one must adjust the marker/blob spacing to be "neither too small nor too large". Recently, Griffith and Luo have proposed an alternative IB approach that models the deformations and stresses of immersed elastic body using a finite element (FE) representation [13]. In their IB/FE approach, the degrees of freedom associated with the tractions are represented on an FE mesh that may be coarser than the fluid grid, and the interaction between the fluid grid and body mesh is handled by placing IB markers at the numerical quadrature points of the FE mesh. When such an approach is generalized to rigid bodies, the conditioning of the linear systems becomes much less sensitive to the marker spacing. Furthermore, the mobility matrix, or approximations of it used for preconditioning, will be smaller and thus easier to fit in memory. We also expect the resulting method to be more accurate because the tractions are represented in a smoother basis. We have recently begun to explore these ideas using the software infrastructure already present in the IBAMR library.

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